2,2,8-Trimethyl-7-prop-2-ynoxychromene

94244-29-8 | DTXSID10241225

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 2730 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.42e-01

Confidence level: 4.97e-01

Nearest Neighbors from the Training Set

Image not found
Ethyl 1-naphthaleneacetate
Measured: 302
Predicted: 425

Image not found
2-Acetylaminofluorene
Measured: 1380
Predicted: 1860

Image not found
3,3'-Dichlorobenzidine
Measured: 22400
Predicted: 1680

Image not found
Imazalil
Measured: 5370
Predicted: 264

Image not found
Pendimethalin
Measured: 5010
Predicted: 4980